201-14674

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August 15, 2003

Ms. Marianne L. Horinko
Acting Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116
Attn: Chemical Right-to-Know Program

Re: HPV Challenge Program, AR-201
Terphenyls, Partially Hydrogenated
CAS Number 61788-32-7

Solutia, Inc., Company Registration Number is pleased to submit the attached Test Plan and Robust Summaries for Terphenyls, Partially Hydrogenated, CAS Number 61788-32-7, as a part of our commitment to the EPA High Production Volume Challenge Program, AR-201.

The attached files are:

1. This cover letter in MS Word 2000
2. Test Plan in MS Word 2000
3. Robust Summaries (IUCLID format) in MS Word 2000

The complete matrix of SIDS data elements, including physical/chemical properties and results of biological and toxicology studies, indicate no additional testing is necessary.

Please contact me at 314-674-1113 if there are any questions relating to this submission.

Regards,

Donald A. Lederer, CHMM
Product Stewardship Manager

HIGH PRODUCTION VOLUME (HPV)

CHEMICALS CHALLENGE PROGRAM

TEST PLAN

For

Terphenyls, Partially Hydrogenated

CAS NO. 61788-32-7

Prepared by:

Solutia Inc. Registration No.

575 Maryville Centre Drive,
St. Louis, Missouri 63141

August, 2003

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EXECUTIVE SUMMARY

Solutia Inc. voluntarily submits the following screening information data and Test Plan covering the chemical, Terphenyls, Partially Hydrogenated (CAS No. 61788-32-7), for review under the Environmental Protection Agency's High Production Volume (HPV) Chemicals Challenge Program.

A substantial amount of data exists to evaluate the potential hazards associated with Hydrogenated Terphenyls. Use of key studies or estimation models, available from data already developed, provide adequate support to characterize the Endpoints in the HPV Chemicals Challenge Program without the need for additional, unnecessary testing.

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TEST PLAN FOR PARTIALLY HYDROGENATED TERPHENYLS

I. INTRODUCTION AND IDENTIFICATION OF CHEMICAL

Under EPA's High Production Volume (HPV) Chemicals Challenge Program, Solutia Inc. has committed to voluntarily compile basic screening data on Partially Hydrogenated Terphenyls (CAS No. 61788-32-7). The data included in this Test Plan provide physicochemical properties, environmental fate, and human and environmental effects of Partially Hydrogenated Terphenyls, as defined by the Organization for Economic Cooperation and Development (OECD). The information provided comes from existing data developed on behalf of Solutia Inc. or found in the published scientific literature and fulfills Solutia's obligation to the HPV Challenge Program.

A. Structure and Nomenclature

The chemical substance identified as "Partially Hydrogenated Terphenyls", the subject of this document, is actually a UVCB mixture with the CAS Registry Number of 61788-32-7. As such, the substance has no recognized chemical structure. The substance is a commercial mixture of several chemical constituents which are derived from a common chemical manufacturing process. This UVCB substance is derived from the partial hydrogenation of an unspecified mixture of the ortho-, meta- and para- isomers of terphenyl, with a lesser amount of quaterphenyl isomers. There is no physical blending of any of the components in the manufacture of this UVCB substance.

Solutia's current commercial products are hydrogenated to a nominal 40% of the theoretical amount of chemical substitution. Essentially all of this UVCB substance is marketed under the commercial trade name of THERMINOL[1] ® 66 Heat Transfer Fluid.

THERMINOL® 66 Heat Transfer Fluid is designated as the test article identification in many of the studies presented in this dossier; in a few cases, data from other commercial and experimental products with similar, but slightly modified compositions, are also presented where appropriate.

Where data are developed using modeling, use of an undefined mixture as the test article is not appropriate. Consequently, the following specific chemical entity was selected as representative of the UVCB mixture. Solutia does not isolate this chemical commercially, but it is believed to be a significant component of the UVCB mixture.

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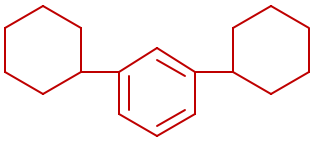
[1] THERMINOL is a registered trademark of Solutia Inc.

Benzene, 1,3-dicyclohexyl-

$C_{18}H_{26}$



B. Manufacturing & Use

Commercial Partially Hydrogenated Terphenyls are manufactured by a single US producer, Solutia Inc. at a single US manufacturing site. The product is also manufactured by Solutia at sites in the United Kingdom and China.

The term "Partially Hydrogenated Terphenyls", is used to describe a commercial mixture of several chemical constituents which, as manufactured by Solutia, are derived from a common chemical manufacturing process. This UVCB substance is manufactured by the partial hydrogenation of an unspecified mixture of the ortho-, meta- and para- isomers of terphenyl, with a lesser amount of quaterphenyl isomers. The composition of the product is a consequence of the reaction chemistry and is not substantially altered through the manufacturing process. There is no physical blending of any of the components to make this UVCB substance. Solutia's current commercial products are hydrogenated to a nominal 40% of the theoretical amount of chemical substitution.

Compositions of the various commercial and developmental products used as test articles in this dossier may vary slightly due to slight differences in the composition of the feedstock which has been hydrogenated. Such differences are small enough that all studies presented can still be considered representative of Partially Hydrogenated Terphenyls, CAS Number 61788-32-7.

The majority of the Partially Hydrogenated Terphenyls manufactured today are marketed as industrial heat transfer fluids under the trade name Therminol® 66 Heat Transfer Fluid. The product is used commercially as a high temperature heat source in various industrial processes. As such it is used in a closed system where the fluid is heated by an external source such as natural gas, then distributed through a closed piping system to one or more heat users in the industrial process. Once heat is

removed from the fluid, it is recirculated back to the heat source. All heat transfer systems using Partially Hydrogenated Terphenyls are liquid systems which operate below the boiling point of the product. This ensures low operating pressure and minimizes the potential for release of vapors to the environment during routine operation.

A small amount of Partially Hydrogenated Terphenyls is also marketed as plasticizers or polymer modifiers.

A TLV of 4.9 mg/m3 (8-hr TWA) has been established for Partially Hydrogenated Terphenyls (ACGIH, 2002). This value has been established to protect against possible dermal or respiratory tract irritation. Only a few employees are involved in the manufacture of commercial Partially Hydrogenated Terphenyls. There is minimal potential for skin or airborne exposure due to the closed nature of the manufacturing process. Eye and skin protection are routinely worn, and respiratory protective equipment is available should airborne exposure limits be exceeded.

II. TEST PLAN RATIONALE

The information obtained and included to support this Revised Test Plan has come from either 1) internal studies conducted by/or for Solutia Inc. (or its predecessor Monsanto Co.), 2) has been extracted from the scientific literature either as primary references or as found in well-accepted, peer-reviewed reference books, or 3) were estimated using environmental models accepted by the US EPA (1999b) for such purposes. This assessment includes information on physicochemical properties, environmental fate, and human and environmental effects associated with Partially Hydrogenated Terphenyls. The data used to support this program include those Endpoints identified by the US EPA (1998); key studies have been identified for each data Endpoint and summarized in Robust Summary form and included in Section VI. of this Dossier.

All studies were reviewed and assessed for reliability according to standards specified by Klimisch *et al* (1997), as recommended by the US EPA (1999a). The following criteria were used for codification:

> 1. Reliable without Restriction - Includes studies which comply with US EPA and/or OECD-accepted testing guidelines, which were conducted using Good Laboratory Practices (GLPs) and for which test parameters are complete and well documented,
>
> 2. Reliable with Restrictions – Includes studies which were conducted according to national/international testing guidance and are well documented. May include studies conducted prior to establishment of testing standards or GLPs but meet the test parameters and data documentation of subsequent guidance; also includes studies with test

parameters which are well documented and scientifically valid but vary slightly from current testing guidance. Also included were physical-chemical property data obtained from reference handbooks as well as environmental endpoint values obtained from an accepted method of estimation (i.e. EPISUITE).

3.Not Reliable – Includes studies in which there are interferences in either the study design or results that provide scientific uncertainty or where documentation is insufficient.

Those studies receiving a Klimisch rating of 1 or 2 are considered adequate to support data assessment needs in this Dossier.

III. TEST PLAN SUMMARY AND CONCLUSIONS

Conclusion: All HPV Endpoints have been satisfied with data from studies that were either well documented, used OECD guideline methods and conducted in accord with GLPs, or were estimated from acceptable estimation modeling programs. Hence, no further testing for any of the HPV Endpoints is deemed necessary, as summarized in Table 1.

In summary:
Physical-chemical property values (Melting Point, Boiling Point, Vapor Pressure, Partition Coefficient and Water Solubility) are measured values which have come from acceptable studies which were classified as "2-Reliable with restrictions".

Environmental Fate values for Transport (Fugacity) were obtained for a significant representative component of the UVCB mixture using a computer estimation – modeling program (EPISUITE, 2002) recommended by EPA; as such, they were designated "2-Reliable with restrictions". The EPISUITE program was unable to estimate Stability in Water (Hydrolysis). Based on the lack of functional groups suggestive of the potential for hydrolysis to occur, it is accepted that Partially Hydrogenated Terphenyls do not hydrolyze appreciably in an aqueous environment. Thus, no additional testing is needed for further confirmation. Biodegradation testing (SCAS and River Die-away) of Partially Hydrogenated Terphenyls has been conducted. The SCAS study was well-documented and was conducted using methodology that preceeded, but is considered consistent with, methodology recommended in OECD test guideline 302. It, thus, has been designated as "2-Reliable with restrictions". The River Die-Away study has been included as Supplemental information. Photodegradation of Partially Hydrogenated Terphenyls has been measured and documented within an internal study coded as "2-Reliable with restrictions".

Ecotoxicity –Acute Fish, Plant (Algal) and Invertebrate Toxicity studies, consistent with OECD test guidance, have been designated as either "1-Reliable without

restriction" or "2-Reliable with restrictions". Additional Supplemental studies have also been summarized for Acute Fish and Invertebrate Endpoints.

Mammalian Toxicity Endpoints (Acute Toxicity, Repeated Dose Toxicity, Ames and Chromosomal Aberration Testing, and Reproductive Toxicity) have all been filled with tests that either conformed directly with OECD test guidance or followed test designs similar to OECD guidance.

The Acute Toxicity Endpoint is supported by an oral rat toxicity study which was conducted according to OECD and GLP guidance and is considered "1- Reliable without restriction".

The Repeated Dose Toxicity Endpoint has been met with a 90-Day Subchronic rat study conducted according to OECD guideline 408 and in accordance with GLPs. It has been codified as "1- Reliable without restriction".

An Ames test, limited by conduct of a single rather than double trial, has been used to fulfill this HPV Endpoint. This study, published in a peer-reviewed journal, is considered "2-Reliable with restrictions". In support of that study and its results, we also provide a similar Ames test, conducted internally according to OECD/GLP guidance with 4 of the 5 Salmonella tester strains called for in OECD study design, as Supplemental information.

An *in vivo* Chromosomal Aberration assay has been used to support its respective Endpoint. Following a study design equivalent to OECD guideline # 475, it has been classified as "1- Reliable without restriction".

The Reproductive Toxicity HPV Endpoint has been filled using a Two-Generation Rat Reproduction study which generally followed OECD test guideline #416 and is considered "2- Reliable with restrictions".

Following is a tabular summary of the Test Plan developed for Partially Hydrogenated Terphenyls.

Table 1. Test Plan Matrix for Partially Hydrogenated Terphenyls

	Info. Avail.	OECD	GLP	Other Study	Estimat. Method	Accept-Able ?	Testing Recomm.
PHYSICAL CHEMICAL							
Melting Point	Y	N	N	N	-	Y	N
Boiling Point	Y	N	N	N	-	Y	N
Vapor Pressure	Y	N	N	N	-	Y	N
Partition Coefficient	Y	N	N	N	-	Y	N
Water Solubility	Y	Y	N	N	-	Y	N
ENVIRONMENTAL FATE ENDPOINTS							
Photodegradation	Y	N	N	N	-	Y	N
Stability in Water	N	-	-	-	-	Y	N
Biodegradation	Y	N	N	Y	-	Y	N
Transport between Environmental Compartments (Fugacity)	Y	N	N	N	Y	Y	N
ECOTOXICITY							
Acute Toxicity to Fish	Y	N	Y	Y	-	Y	N
Acute Toxicity to Aquatic Invertebrates	Y	Y	Y	Y	-	Y	N
Toxicity to Aquatic Plants	Y	N	N	N	-	Y	N
MAMMALIAN TOXICITY							
Acute Toxicity	Y	Y	Y	Y	-	Y	N
Repeated Dose Toxicity	Y	Y	Y	N	-	Y	N
Genetic Toxicity – Mutation (Ames)	Y	Y	Y	Y	-	Y	N
Genetic Toxicity – Chromosomal Aberrations	Y	Y	Y	N	-	Y	N
Developmental Toxicity	-	-	-	-	-	-	-
Reproductive Toxicity	Y	Y	Y	N	-	Y	N

Y = Yes; N = No; - = Not applicable

III. DATA SET SUMMARY AND EVALUATION

The key studies used in this assessment to fulfill the HPV requirements have been placed in an Endpoint-specific matrix, and further discussed below. Robust Summaries for each study referenced can be found in Section VI of this Dossier.

A. Chemical/Physical Properties

Table 2. Selected Chemical/Physical Properties of Partially Hydrogenated Terphenyls

Chemical	Boiling Pt. (°C.)	Melting Pt.(° C.)	Vapor Pressure (hPa @ 25 °C)	Water Solubility (mg/L)	Partition Coefficient (Log Kow)
Partially Hydrogenated Terphenyls CAS No. 61788-32-7	359	-32 (pour point)	0.002666	< 0.06	6.13

All HPV Endpoints for Physical-Chemical Properties have been completed with reliable information, either taken from studies which have been designated as "2-Reliable with restrictions", are included in the Robust Summary section of this Dossier.

In summary, these data indicate that Partially Hydrogenated Terphenyls is a liquid at room temperature and has a very low vapor pressure. It has a moderately high octanol:water partition coefficient and very low solubility in water.

Conclusion – Adequate reference values are available to provide needed information on the Physical-Chemical Properties associated with Partially Hydrogenated Terphenyls. Therefore, no additional data development is needed for these HPV Endpoints.

B. Environmental Fate and Biodegradation

Both a Semi-Continuous Activated Sludge (SCAS) test and a River Die-Away test have been conducted with Partially Hydrogenated Terphenyls. While conducted prior to inception of standardized international guidelines for **Biodegradability** testing and GLPs, these studies followed similar standards for conduct subsequently codified into OECD guideline 302 and GLP documentation. They are considered "2-Reliable with restrictions". Both studies have been summarized in the Robust Summary section of this

Dossier. The SCAS study has been selected to fulfill this HPV Endpoint and is cited in Table 3 below.

No/little information could be located regarding Stability in Water (Hydrolysis) and Transport (Fugacity) for Partially Hydrogenated Terphenyls following an extensive literature search. We have incorporated the use of the estimation models found in EPISUITE (2002) for determination of **Fugacity** for a major component (1,3-dicyclohexyl benzene) of Partially Hydrogenated Terphenyls (PHT)s, as PHTs is a UVCB substance without a defined structure. The values derived are cited with the Robust Summaries and also are included in Table 3 and has been judged as "2-Reliable with restrictions". No Hydrolysis values could be calculated using EPISUITE (2002) for either the mixture or a major component (dicyclohexyl benzene), as these chemicals have only saturated/unsaturated aromatic rings and no functional groups. These structures are consistent with those listed in Lyman et al, 1990) as "Generally Resistant to Hydrolysis". Thus, "[t]esting for Stability in Water is not needed for substances generally recognized to have molecular structures or possess only functional groups that are generally known to be resistant to hydrolysis" (OECD, 2002).

Table 3. Environmental Fate and Biodegradation Parameters for Partially Hydrogenated Terphenyls

Chemical	Biodegradation Rate	Stability in Water (T ½ days @ 25 deg.)	Fugacity (%)	Photodegrad. Rate (T ½)
Partially Hydrogenated Terphenyls CAS No. 61788-32-7	35 %	Not susceptible to Hydrolysis	Air – 0.2 Water – 3.6 Soil – 27.5 Sediment – 68.7	86 days

The Environmental Fate and Biodegradability of Partially Hydrogenated Terphenyls can be summarized as follows.

Partially Hydrogenated Terphenyls would not be expected to normally enter the aquatic environment, as they are intended to be used in enclosed systems. However, their limited entry could be envisioned after incidental spills and equipment leakage. Thus, based on Fugacity modeling, their environmental fate is expected to focus on the soil and sediment as main environmental target compartments. As Partially Hydrogenated Terphenyls are not readily hydrolysable, have exceedingly low water solubility characteristics and appear to undergo limited photolysis, their presence in aqueous or atmospheric compartments is minimal. Partially Hydrogenated Terphenyls can be expected to partition mostly to the soil or sediment. As part of the soil or sediment, Partially Hydrogenated Terphenyls will degrade; while not Readily Biodegradable, significant biodegradation has been established in inherent biodegradation studies (SCAS and River Die Away).

Conclusion – Adequate studies are available to provide needed information for the HPV Designated Environmental Properties associated with Partially Hydrogenated Terphenyls. No further testing is planned.

C. Aquatic Toxicity

Sufficient information is available to characterize the acute toxicity of Partially Hydrogenated Terphenyls to algae, invertebrates and fish. An acute fish study, following OECD test guidance has been conducted on F. Minnows and is considered "2-Reliable with restrictions". A similar study with R. trout has been provided as Supplemental information. A Robust Summary has been prepared for these studies and the F. Minnow study cited in Table 4.

A well-conducted study summarizing the effects of Partially Hydrogenated Terphenyls in *D. magna* and has been used to fulfill the Acute Invertebrate Toxicity Endpoint. It has been judged as "1-Reliable without restriction".

An acute Algal study fulfills the Acute Plant Toxicity HPV Endpoint. While not conducted specifically to meet OECD guidelines, this study used methodology recommended by the US EPA Committee of Methods for Toxicity Testing with Aquatic Organisms (EPA, 1975). These recommendations are consistent with OECD guidelines. Hence, it has been designated as "2- Reliable with restrictions", selected for development of Robust Summaries, and is cited in Table 4.

Several of the acute aquatic studies referenced above used nominal test levels which exceeded the very low (<0.06 ppm) water solubility limit for Partially Hydrogenated Terphenyls. In review of the study data, no treatment-related toxicity was discernable at test levels which clearly exceeded solubility limits. Thus, it is scientifically rational to conclude that the EC50/LC50 for Partially Hydrogenated Terphenyls is in excess of this aqueous solubility limit. Further efforts to derive a toxicity value above the solubility limits of this substance would provide no meaningful value useful in the assessment of environmental risk.

Table 4. Aquatic toxicity parameters for Partially Hydrogenated Terphenyls

Chemical	Fish LC 50 (mg/L)	Invertebrate EC50 (mg/L)	Algae EC50 (mg/L)
Partially Hydrogenated Terphenyls CAS No. 61788-32-7	> 0.06 (limit of solubility)	>1.34	> 0.06 (limit of solubility)

Conclusion – An adequate study is available to meet each of the three Acute Aquatic Toxicity Endpoints for Partially Hydrogenated Terphenyls. No additional testing is necessary for this completed HPV Endpoint category.

D. Mammalian Toxicity Endpoints

A summary of toxicity data used to fulfill the HPV Endpoints for Mammalian Toxicity is found in Table 5. Each report citation has been further summarized in the Robust Summary section of this Dossier.

Table 5. Mammalian Toxicity of Partially Hydrogenated Terphenyls

Chemical	Acute Oral LD50 (rat)	Repeat Dose Toxicity	Ames Test	Chromosomal Aberrations	Reproductive Toxicity
Partially Hydrogenated Terphenyls CAS No. 61788-32-7	> 10,000 mg/kg	(91-day Rat oral) NOEL =200 ppm	Non-mutagenic: TA 1535, 1537, 1538, 98, 100 with and w/out S9	(in vivo rat bone marrow) Non-mutagenic	(2-Gen. rat) NOAEL = 1000 ppm

1.0 Acute Toxicity

Results of an acute oral toxicity study with Partially Hydrogenated Terphenyls fulfill the HPV Acute Toxicity Endpoint. This study was conducted as a Limit Test according to OECD Test Guidelines and GLP guidance and provides sufficiently reliable, documented information to be classified as "1- Reliable without restriction".

Thus, Partially Hydrogenated Terphenyls is considered to be practically non-toxic after administration by acute oral dosing.

Conclusion – A study of sufficient quality is available to assess the Acute hazard associated with Partially Hydrogenated Terphenyls. Therefore, no additional data development is needed for the Acute Toxicity HPV Endpoint.

2.0 Repeated Dose Toxicity

Partially Hydrogenated Terphenyls has been adequately tested in a subchronic rodent study to define its Repeated Dose toxicity. This study is cited in Table 5 and summarizes a 91-day subchronic rat study by the oral route. This study was conducted using a study design according to OECD Test Guideline 408, and conducted under GLP auspices. Hence, it is considered "1- Reliable without restriction". In all cases, no evidence of an effect on the male or female reproductive organs (including testes) was observed.

Conclusion - The Repeated Dose HPV Endpoint for Partially Hydrogenated Terphenyls has been fulfilled with a well-conducted and documented 90-Day Subchronic study in rats deemed "1- Reliable without restriction". No further testing is needed for completion of information related to the Repeat Dose HPV Endpoint.

3.0 Mutagenicity and Chromosomal Aberrations

3.1 Ames/Point Mutation Testing

When tested in two standard Ames assays for point mutations, Partially Hydrogenated Terphenyls elicited no mutagenic response in any of the *S. Typhimurium* tester strains employed, either with or without inclusion of metabolic activation (Table 5). The published, peer-reviewed literature study (Clark et al., 1979) has been classified as "2-Reliable with restrictions" due to its use of fewer replications than recommended in OECD study guide # 471. However, an additional, well-documented Ames assay (Solutia study no. DA-78-184-see Robust Summary), conducted internally with 4 of the 5 *Salmonella* tester strains included in the OECD test guidance, validates the conclusion of a lack of mutagenicity reported in the literature with Partially Hydrogenated Terphenyls. Both studies are summarized in the Robust Summary section of this Dossier.

Thus, it is concluded that adequate testing of sufficient quality has been performed on Partially Hydrogenated Terphenyls to evaluate the Ames Test (Point Mutation) HPV requirement; no further testing is needed for this Endpoint.

3.2 - Chromosomal Aberrations

Partially Hydrogenated Terphenyls has been tested *in vivo* for induction of Chromosomal Aberrations in rat bone marrow cells. This study followed OECD Guideline # 475 and was conducted following GLPs. Thus this study is considered as "1-Reliable without restriction". No mutagenic activity was observed.

The HPV Chromosomal Aberration Endpoint for testing of Partially Hydrogenated Terphenyls has, thus, been fulfilled with an adequately conducted and documented *in vivo* study; no further testing is needed.

4.0 Reproductive Toxicity

Of direct relevance to completion of the Reproductive Toxicity Endpoint for this HPV assessment with Partially Hydrogenated Terphenyls, is identification of a well documented 2-Generation rat Reproduction Toxicity study conducted in general accord with OECD Guideline 416. This study has been assessed as "2- Reliable with restrictions". It has been summarized in the Robust Summary section of this Dossier and is included in Table 5.

No evidence of reproductive toxicity was observed in this study nor were morphological effects of either male or female reproductive organs observed in this study or following subchronic testing (Table 5).

In conclusion, the Reproductive Toxicity HPV Endpoint has been fulfilled using a well documented and conducted 2-Generation Reproductive study which has been assessed as "2- Reliable with restrictions". Thus, the data requirements for this HPV Endpoint have been met and no further testing is required.

V. REFERENCES

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Clark, CR, TC Marshall, BS Merickel, A Sanchez, DG Brownstein and CH Hobbs, 1979. Toxicological Assessment of Heat Transfer Fluids Proposed for Use in Solar Energy Applications. Toxicol. Appl. Pharmacol. 51:529-535.

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OECD, 2002. Organization of Economic Cooperation and Development. Existing Chemicals Programme. SIDS Dossier on the HPV Chemicals (latest draft – May, 2002).

US EPA. 1975. Committee of Methods for Toxicity Testing with Aquatic Organisms. Methods of acute toxicity tests with fish, macroinverterates and amphibians. US EPA Ecol. Res. Ser. 660/3-75009.

US EPA, 1998. Guidance for meeting the SIDS requirements (The SIDS Guide). Guidance for the HPV Challenge Program (11/31/98).

US EPA, 1999a. Determining the adequacy of existing data. Guidance for the HPV Challenge Program (2/10/99).

US EPA, 1999b. The use of structure-activity relationships (SAR) in the High Production Volume Chemicals Challenge Program. OPPT, EPA.

VI ROBUST STUDY SUMMARIES -

A IUCLID Data Set for Hydrogenated Terphenyls is Appended

I U C L I D

Data Set

Existing Chemical	:	ID: 61788-32-7
CAS No.	:	61788-32-7
EINECS Name	:	Terphenyl, hydrogenated
EC No.	:	262-967-7
TSCA Name	:	Terphenyl, hydrogenated

Producer related part

Company	:	Solutia Inc.
Creation date	:	17.03.2003

Substance related part

Company	:	Solutia Inc.
Creation date	:	17.03.2003
Status	:	
Memo	:	
Printing date	:	28.07.2003
Revision date	:	
Date of last update	:	28.07.2003
Number of pages	:	28
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

Reliability : (1) valid without restriction
24.06.2003

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	
Purity	:	> 98 - % v/v
Colour	:	
Odour	:	

Test substance : Commercial Grade of greater than 98% purity. Consists of approximately 40% Partially Hydrogenated Terphenyls (80-85%) and Quaterphenyls (15-20%).

24.06.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	-32 - °C
Sublimation	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	As this material is a liquid at room temperature, the mp has been expressed as the pour point.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

24.06.2003 (1)

2.2 BOILING POINT

Value	:	359 - °C at
Decomposition	:	
Method	:	
Year	:	2003
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

24.06.2003 (1)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.002666 - hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	1985
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Gas saturation technique.
Remark	:	Reported as 0.002 @ mm Hg 25 deg C.
Test substance	:	MXP-2020, a precommercial sample of THERMINOL 66 of essentially same purity of approx. 98%.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

24.07.2003 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	6.13 - at 23 °C
pH value	:	-
Method	:	
Year	:	1977
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Partition coefficient was determined via a direct partition experiment. At least two concentrations of the test substance were prepared in 100 ml of n-octanol. The n-octanol test solutions were combined with 500 ml purified water in a 1-l glass bottle at room temperature (ca. 25 deg. C) and shaken for 48 hours. Shaken mixtures were allowed to separate for 1 week in the dark. Concentrations of the test substance in each phase were determined by gas chromatography with dual flame-ionization detectors (GC-FID/FID). The partition coefficient (P) was calculated using the following equation: P = Co/Cw where Co and Cw are the concentrations of the test substance in n-octanol and water, respectively.
Result	:	Reported as 1.36x10E6.
Test substance	:	Santosol 340
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

24.07.2003 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	< .06 - mg/l at 23 °C
pH value	:	-
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	OECD Guide-line 105
Year	:	1995
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Value cited was maximum value, as the methodology would not allow attempts for detection at even lower levels.
Test substance	:	Santotherm 66
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

24.07.2003 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Deg. product	:	
Method	:	other (measured)
Year	:	1982
GLP	:	no data
Test substance	:	other TS
Method	:	Direct analysis of photodegradation in sunlight. A 50 mg/L aqueous concentration using acetonitrile solvent was added to duplicate quartz tubes, sealed and exposed to sunlight (> 100 hrs over 15 day test period) at ave. temp. of 62 deg. F. Test sample was measured at intervals of 0, 2, 5, 9 and 15 days after exposure. Darkened tubes were also analyzed and amount of degradation subtracted from light-exposed tubes to define the degree of photolysis. Analysis conducted using GC -FID.
Result	:	T 1/2 = 86 days
Test substance	:	MXP-2020, an precommercial sample of THERMINOL 66 of similar purity of approx. 98%.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

28.07.2003 (5)

3.1.2 STABILITY IN WATER

Remark	:	Test material is not susceptible to hydrolysis.

28.07.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	.229 % (Fugacity Model Level I)
Water	:	3.57 % (Fugacity Model Level I)
Soil	:	27.5 % (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	68.7 % (Fugacity Model Level II/III)
Method	:	other:Calculation based on EPISUITE
Year	:	2003
Method	:	Level III fugacity based model, EPISUITE 3.10. Default values were assumed for environmental compartment descriptions, dimensions and properties, advective and dispersive properties. Chemical -specific modeling parameters as calculated by the model were: molecular weight= 242.41 g/mol, vapor pressure = 0.00012 hPa at 25 deg. C, log Kow = 7.63,

melting point = 77.77 deg. C. and a Henry's Law constant of 0.00292 atm-m3/mol. Half-lives calculated by the model based on the properties of the test substance were: air half-life = 8.29 hr, water and soil half-lives = 900 hr, and sediment half-life = 3600 hr. Emissions were assumed to be equal to air, water, and soil.

Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major component of Partially Hydrogenated Terphenyls) with a SMILES notation of C(CCCC3)(C3)c(cccc1(C(CCCC2)C2))c1.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

28.07.2003 (6)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other: municipal sewage treatment plant
Concentration : 10 g/l related to Test substance
related to
Contact time : 9 month
Degradation : 35 - 1 (±8.6) % after 24 hour(s)
Result :
Deg. product :
Method : other: Semi-Continuous Activated Sludge (SCAS)
Year : 1971
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : 9 month SCAS test generally consistent with OECD guideline 302, 4 test periods of 4 to 29 days, 24-h cycle of draw and fill, weekly analyses of parent material using UV absorbance, while metabolites were quantified using GC-FID, 10 mg test material was added per cycle, activated sludge mixed liquor from municipal sewage treatment plant was inocula, a series of 3 hexane off-gas scrubbers were used to catch volatiles.

Result : For time period 1, mean and 95% CI disappearance rate was 19.5 +/- 20.8%, for period 2 it was 55.0 +/- 12.9%, for period 3 it was 25.0 +/- 81.2% and for period 4 it was 48.6 +/- 6.9%. Overall mean daily disappearance rate was 35.1 +/- 8.6%. GC analyses showed that the several peaks that make up the test material degraded at varying levels. No volatile losses were reported.

Test substance : HB-40
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

11.07.2003 (7)

Type : aerobic
Inoculum : other: Meramec River water
Contact time :
Degradation : 68 - (±) % after 50 day(s)
Result :
Deg. product :
Method : other: River-Die Away test
Year : 1971
GLP : no

Test substance	:	as prescribed by 1.1 - 1.4
Method	:	River water was obtained from the Meramec River near St. Louis, Missouri, USA. Settled water (2 days) was added (200 mL) to 16-oz. wide-mouth bottles. Distilled water controls (with test substance) were prepared similarly to assess sorption to glass and volatilization. Test material was added in 5 microliter volumes prepared with 4% (W/V) ethanol. Bottles were sealed with foil-lined caps and stored at room temperature in the dark for up to 50 days. A positive control (LAS Reference #2 - Dodecene-1) was prepared similarly and used to verify the biological activity. Periodically, chemical analyses were made by sacrificing a bottle containing test material and a control. Three 50-mL aliquots of hexane were injected into the bottle, the bottle vigorously shaken, and the phases allowed to separate. The three portions of hexane were collected, concentrated to 10 mL using a Kudema-Danish concentrater, transferred to a 10 mL cell and the UV absorption determined. Recoveries of spiked samples for the test substance were 91.6%.
Result	:	Losses from the distilled water control were 13%. Test material was reduced by 68% in 21 days and by 81% (net loss of 68%) in 50 days.
Test substance	:	HB-40
Reliability	:	(2) valid with restrictions Supplemental information which indicates considerable biological breakdown in the environment.

11.07.2003 (7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> .06 -
Limit test	:	yes
Analytical monitoring	:	no
Method	:	other: US EPA 660/3-75-009
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : This study followed US EPA guideline 660/3-75-009. 1975. Committee on Methods for Toxicity Tests with Aquatic Organisms. Fathead minnows were obtained from a fish hatchery, held in culture tanks for two weeks under 16 hrs light, 8 hrs dark. Fish were fed commercial fish food until 48 hr before the test. Fish had a mean weight and length of 0.46 g and 30.4 mm, respectively. Static bioassay was performed in a 40 L glass aquaria containing 30 L of laboratory well water and 10 (ten) fish per concentration. Antimycin a was used as a positive control. Water quality of test dilution at test initiation was: DO 9.3 mg/L, pH 7.8-8.2, total hardness of 255 mg/L CaCO3, total alkalinity of 368 mg/L CaCO3. Test water was maintained at 22 +/- 1 deg. C in a water bath. Fish were held without food for 48 hrs before testing and were not fed during the test. Based on finding no toxicity at 1000 mg/L in a range-find test, a definitive test was conducted at 1,000 mg/L nominal test material. A test concentration was prepared by adding test material directly to the test vessel; no meaurements of test material were taken during the test. An oily film was observed in the test vessels during the study. Across all test vessels, DO varied between 5.2 to 8.5 mg/L, pH ranged from 7.3-8.3, temperature remained close to 22 deg. C.

Result : No control mortalities were observed and only 10% deaths were seen in the 1000 mg/L Limit Test dose after 96 hours of testing. Thus the 96-h LC50 was > 1000 mg/L nominal. As the water solubility of the test agent is less than 0.06 mg/L., then the LC50 correctly stated is > 0.06 mg/L.

Test substance : Therminol 66

Reliability : (2) valid with restrictions
While the nominal dose level used in this study well exceeded the water solubility of Therminol 66, it can reasonably be concluded that the 96-h EC50 is in excess of the water solubility limit, as the nominal concentration proved to produce only limited (10% deaths) toxicity.

Flag : Critical study for SIDS endpoint

28.07.2003 (8)

Type	:	static
Species	:	Salmo gairdneri (Fish, estuary, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> .06 -
Limit test	:	yes
Analytical monitoring	:	no
Method	:	other: US EPA 660/3-75-009
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : This study followed US EPA guideline 660/3-75-009. 1975. Committee on

Methods for Toxicity Tests with Aquatic Organisms. Rainbow trout were obtained from a fish hatchery, held in culture tanks for two weeks under 16 hrs light, 8 hrs dark. Fish were fed commercial fish food until 48 hr before the test. Fish had a mean weight and length of 1.02 g and 39.1 mm, respectively. Static bioassay was performed in a 5 gal. glass aquaria containing 15 L of laboratory well water. Ten (10) fish per test concentration level were used. Antimycin A was tested as a positive control. Water quality of test dilution at test initiation was: DO 8.9 mg/L, pH 7.8, total hardness of 240 mg/L CaCO3, total alkalinity of 360 mg/L CaCO3. Test water was maintained at 12 +/- 1 deg. C in a water bath. Fish were held without food for 48 hrs before testing and were not fed during the test. Based on finding no toxicity at 1000 mg/L in a range-find test, a definitive test was conducted at 1,000 mg/L nominal test material. A test concentration was prepared by adding test material directly to the test vessel; no meaurements of test material were taken during the test. An oily film was observed in the test vessels during the study. Across all test vessels, DO varied between 5.8 to 7.3 mg/L, pH ranged from 7.3-8.3, temperature remained at 12 deg. C.

Reliability : (2) valid with restrictions
Provided as Supplemental information. While the nominal dose level used in this study well exceeded the water solubility of Therminol 66, it is reasonable conclude that the 96-h EC50 is in excess of the water solubility limit (0.06 mg/L), as the nominal concentration proved to produce only limited (10% deaths) toxicity.

28.07.2003 (9)

Type : other
Species : other: calculated
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = .00092 - calculated
Method : other: calculation based on ECOSAR
Year : 2003
GLP : no
Test substance : other TS

Method : 96-Hr Fish LC50 calculation using ECOSAR, from the USEPA. Value was calculated using a calculated log Kow of 7.63. The SAR for neutral organics was employed.
Remark : Provided as Supplemental Information to this HPV data package.
Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major component of Partially Hydrogenated Terphenyls) with a SMILES notation of C(CCCC3)(C3)c(cccc1(C(CCCC2)C2))c1.

28.07.2003 (10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : >= 1.34 - measured/nominal
EC50 : >= 1.34 - measured/nominal
Limit Test : yes
Analytical monitoring : yes
Method : OECD Guide-line 202
Year : 1996
GLP : yes
Test substance : other TS

Method	:	Twenty < 24-h old D. magna Straus were tested at 20 +/- 1 deg. C in a series of four replicates per test concentration. The Limit Test was conducted at 1.34 mg/L and included clean water and solvent (ethoxylated triglyceride at 150 mg/L) controls. Stock solutions had a few white dust-looking particles floating on their surface. Tests were conducted using reconstituted distilled water. Water was reconstituted with CaCl2, MgSO4, NaHCO3 and KCl. At test initiation, the pH was 7.97. DO was at 23.8% of saturation, specific conductance was at 680 micro-siemens, hardness was 262 mg/L, alkalinity was 34 mg/L. Test concentrations were measured using HPLC. Daphnids were not fed during the test. Tests were conducted in 1 fluid ounce plastic cups containing 25 mL of solution. Dissolved oxygen, temperature and pH were monitored at the beginning and end of the test. At test initiation, the test substance concentration was 1.34 mg/L and at 28 hr it was 1.29 mg/L. A photoperiod was not specified in the report. However, as this study was conducted in late July/early August in St. Louis Mo. the average photoperiod in that location is approximately 16-h light,8-h dark.
Result	:	Limit Test 48-h EC50 = >1.34 mg/L; 24-h EC50 >1.34 mg/L. NOEC => 1.34 mg/L. There were no immobilizations reported in either control or in vessels with test substance at either 24 or 48 hrs. At test initiation, pH ranged from 7.96 to 8.03, DO ranged from 17.3 to 23.4% of saturation and temperature ranged from 22 to 23 deg. C. At 48 hrs, pH ranged from 7.77 to 8.02, DO ranged from 20.1 to 22.7% of saturation, and temperature ranged from 20.4 to 21.6 deg. C.
Test substance	:	THERMINOL 66
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint
24.07.2003		(11)

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	< .056 -
EC50	:	= .1 -
Method	:	other
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method	:	Followed guidance according to EPA 660/3-75-009. Ten < 24-h old D. magna Straus were tested at 20 +/- deg. C. in a series of two replicates per test concentration. Test concentrations were 0.056 (level of solubility), 0.10, 0.18, 0.32 and 0.56 mg/L, plus clean water and solvent (acetone) controls. Tests were conducted using well water from Columbia, MO. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 250-mL beakers containing 200 mL of solution. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test. Water quality was measured for dissolved oxygen, pH, ammonia, and temperature and no significant changes were observed in any parameter during the test. The estimated EC50 and 95% confidence limits were determined using EPA statistical procedures (probit analysis).
Remark	:	Supplemental information
Result	:	48-h EC50 (95% CL) = 0.10 (0.075-0.13) mg/L; 24-h EC50 (95% CL) = 0.70 (0.49-1.0); NOEC = < 0.056 mg/L.; At 24-h, there were no mortalities in controls or the lower two test concentrations. Clumping of daphnids was observed at the highest 3 concentrations. At 48-h, there were no mortalities (0/10; 0/10) in controls. There were partial mortalities in the lower three test concentrations [2/10;2/10 @ 0.056 mg/L; 4/10,5/10 @ 0.10 mg/L;8/10, 10/10 @0.18 mg/L]and 100% mortality in the highest two (0.32

& 0.56 mg/L) concentrations. Mortalities followed a dose-response pattern.

Test substance : Therminol 66
Reliability : (2) valid with restrictions
11.07.2003 (12)

Type : other: Calculation
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = .00145 - calculated
Method : other: calculation using ECOSAR
Year : 2003
GLP : no
Test substance : other TS

Method : 48-Hr Daphnia LC50 calculation using ECOSAR, from the USEPA. Value was calculated using a calculated log Kow of 7.63. The SAR for neutral organics was employed.
Remark : Provided as Supplemental Information to this HPV data package.
Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major component of Partially Hydrogenated Terphenyls) with a SMILES notation of C(CCCC3)(C3)c(cccc1(C(CCCC2)C2))c1.
28.07.2003 (10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint : other: chlorophyl a, cell number
Exposure period : 96 hour(s)
Unit : mg/l
EC50 (chlorophyl a) : > .06 -
EC50 (cell number) : > .06 -
Limit test :
Analytical monitoring : no
Method : other: US EPA, 1971.
Year : 1979
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : The study followed methods outlined in USEPA, 1971. Algal Assay Procedure: Bottle Test. National Eutrophication Research Program. Pacific Northwest Water Laboratory, Corvallis, OR. Cultures were incubated at 24 +/- deg. C under 4000 lux illumination during a 24-h/d photoperiod. Triplicate culture flasks were employed for each of the test concentrations and controls used. Nominal test concentrations were 10, 32, 56, 100 and 320 mg/L. Both clean water and solvent controls were included. Dimethylformamide (DMF) was used as a cosolvent (0.05 mL per test flask). Test material was dissolved in DMG and directly added to the test vessels. Initial cell counts were ~ 20,000 cells/mL. chlorophyll a was measured using a Turner Model 111 fluorometer. Cell counts were made using a hemacytometer and a Zeiss Standard 14 compound microscope. Specifics of the culture medium were not provided other than stating that test medium was based on USEPA guidance. Results were analyzed using the Student's t test. PH was maintained between 7.2 and 7.4 during the test.
Result : Chlorophyll a
96-h EC50 (95% CI) = 44 (1-1586) mg/L.
24-h EC50 (95% CI) = >320 mg/L
48-h EC50 (95% CI) = >320 mg/L
72-h EC50 (95% CI) = >100 < 320 mg/L.

Cell number
96-h EC50 (95% CI) = 56 (4-743) mg/L.

As the water solubility of THERMINOL 66 is less than 0.06 mg/L, this level was exceeded in both phases of this study. However, as there were no toxic effects observed at the lowest dose tested, it can be concluded that the EC50 > 0.06.

Test substance : Therminol 66
Reliability : (2) valid with restrictions
All test levels exceeded the water solubility limit of Therminol 66 of less than 0.06 mg/L. However, the lowest dose levels in this study did not produce a treatment-related effect. Thus, it can be concluded that no effects were seen up to the level of water solubility for this material.
Flag : Critical study for SIDS endpoint
28.07.2003 (13)

Species : other algae
Endpoint : other: calculation for green algae
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = .00125 - calculated
Method : other: calculation based on ECOSAR
Year : 2003
GLP : no
Test substance : other TS

Method : 96-Hr Algae LC50 calculation using ECOSAR, from the USEPA. Value was calculated using a calculated log Kow of 7.63. The SAR for neutral organics was employed.
Remark : Provided as Supplemental Information to this HPV Package.
Test substance : A representative structure of 1,3-Dicyclohexyl benzene (a major component of Partially Hydrogenated Terphenyls) with a SMILES notation of C(CCCC3)(C3)c(cccc1(C(CCCC2)C2))c1.
28.07.2003 (10)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	other: Limit Test
Value	:	> 10000 - mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	
Doses	:	10,000 mg/kg
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1979
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	A single group of 5 male and 5 female fasted SD rats were administered 10,000 mg/kg test material via gavage and observed for 15 days. Twice daily examinations were made for mortality and signs of toxicity. Body weights were recorded on the first day of testing and weekly thereafter. Food and water were given ad libitum. Temperature, humidity and light cycle were controled. At the end of the study, all survivors were given a full necropsy.
Result	:	No deaths occurred at the single dosage level tested of 10,000 mg/kg. Signs of toxicity included: hypoactivity, diarrhea and feces - and urine-stained fur. All animals were normal at necropsy.
Test substance	:	Commercial grade HB-40 of > 98% purity.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

24.06.2003 (14)

Type	:	other: Limit Test
Value	:	> 24000 - mg/kg bw
Species	:	rat
Strain	:	Fischer 344
Sex	:	female
Number of animals	:	
Vehicle	:	other: undiluted
Doses	:	no data available
Method	:	other
Year	:	1979
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Female F344 rats, 12-14 weeks old, were fasted overnight and then dosed by gavage with undiluted test material. No dosage exceeded 24 g/kg bw. Five rats per treatment group were tested using dosages spaced at 0.1 log increments. Animals were maintained at 20 +/- 2 deg. C, 12-hr light:dark cycle and had water and food provided ad libitum. Daily observations for clinical signs were taken throughout the 14-day test period; body weights were recorded prestudy and weekly thereafter. Gross pathological examinations were carried out on selected animals which survived the highest dose tested. As this study resulted in a Limit Test, no LD50 calculation, using the method of Deichmann and LeBlanc, was made.
Result	:	LD50 value was determined to be above the highest dose tested of 24,000 mg/kg. Other than diarrhea during the first 24-hrs, no other clinical signs of

toxicity were reported. No evidence of gross pathological effects were reported.

Test substance : Test material was referenced as commercial grade THERMINOL 66, obtained from Monsanto Co.

Reliability : (2) valid with restrictions
This information is supplied as Supplemental to a previously reported Limit Test by the oral route for THERMINOL 66.

26.06.2003 (15)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	91 days
Frequency of treatm.	:	daily
Post exposure period	:	none
Doses	:	50, 200, 2000 ppm
Control group	:	yes
NOAEL	:	>= 200 - ppm
LOAEL	:	>= 2000 - ppm
Method	:	OECD Guide-line 408 "Subchronic Oral Toxicity - Rodent: 90-day Study"
Year	:	1984
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : Groups of 12 male and 12 female SD rats (approx. 4 wks old) were administered a diet admixed directly with test material for 91 days. Levels of test material were verified during weekly diet analysis. All rats were examined for morbidity and mortality twice daily. Body weights and food consumption were measured weekly, and detailed signs of toxicity recorded. Humidity, temperature and lighting were controled. Clinical pathology for the following indices were measured for 10 rats/sex/group after 1 and again after 3 months on test: Hematology - HCT, HGB, RBC, WBC, Platelets, erythrocyte morphology and differ. leukocytes; Serum Chemistry - Ca, In. Phos, CL, Na, K, GLU, ALT, AST, BUN, Albumin, globulin, T. Prot., Creat., T. Bili and GGTP. An ophthalmoscopic

examination was given to all rats prior to study start and at study term. At the end of the study, all rats were given a necropsy and organ weights and body:organ weight ratios recorded for: brain, kidney, liver, testes and adrenals. Histopathological examination of a full set of tissues and organs, including ovaries, testes,adrenals, aorta, bone, marrow, femur, brain, esophagus, eyes, exorbital lacrimal gland, heart, intestines (6 sections), kidneys, liver, lungs, lymph nodes, mammary gland, uterus, pancreas, pituitary, prostate, salivary gland, seminal vesicles, skel. muscle, skin, spinal cord, nerve, spleen, stomach, thymus, thyroid/parathyroid, trachea, epididymides and all gross lesions were given to all rats in the control and high dose group. Livers, Lungs and kidneys from all mid and low dose animals were also examined microscopically. Statistical analysis of body weights, food consumption, growth rates, clinical pathology, organ weights and ratios were performed using Leven's Test for homogeneity and ANOVA followed by Terpstra-Jonckheere test and Dunnett's test for group-wise comparison.

Remark : Based on food consumption and body weight data conversion factors, the dosages of test articles employed in this study were approximately 150, 15 and 3.5 mg/kg/d.

Result : The NOAEL for this study is considered to be 200 ppm.

The following treatment-related effects seen at 2000 ppm were minimal in nature: small decreases in body weight in males (2.7%) and females (6-7%). Small but statistically significant decreases in hemoglobin, hematocrit and erythrocyte count were observed in high dose males, but not females, at the 1 month interval, but were no longer statistically significant at study termination. A statistical increase in platelet counts was seen in this study group at both the 1 and 3 month interval.
Cholesterol and albumin were elevated in high dose males after 3 months (cholesterol also after 1 mo.). Both males and females exhibited increased absolute kidney and liver weight increases as well as corresponding increased organ/body and organ/brain weight ratios. Microscopic evaluation resulted in no morphological evidence of a direct toxicopathologic effect of treatment. High dose males, but not females, had an increased incidence (but similar level of severity) of a spontaneously occurring regenerative renal lesion also present in control male rats. The pathological significance of this finding was deemed unclear. No treatment-related effects were seen on male or female reproductive organs.

Test substance : Therminol 66
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
11.07.2003 (16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium tester strains TA 1535, 1537, 1538, 98 and 100
Test concentration : 1 to 10,000 ug/plate
Cycotoxic concentr. : not reported; none apparently seen up to highest dose tested
Metabolic activation : with and without
Result : negative
Method : other: Ames et al. 1975. Mutat. Res. 31:347-364.
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Method of testing and evaluation used the procedures described in Ames et al, 1975, Mutat. Res. 31:347-354. Test samples diluted in dimethyl sulfoxide were prepared to give final concentrations ranging from 1 to 10,000 ug/plate in 0.1 ml. Negative and positive controls (MNNG, 2-AAF

abd 9-AA) were used. Each of 5 Salmonella tester strains, TA1535, 1537, 1538, 98 and 100 were tested in replicate plates with and without inclusion of liver homogenates from Arochlor 1254-treated male rats as the activation system.

Result : No significant mutagenic activity seen in any of the Salmonella tester strains used, with or without metabolic activation.
Test substance : Commercial grade sample of THERMINOL 66, obtained from Monsanto Co.
Reliability : (2) valid with restrictions
No data shown in peer-reviewed publication; however, raw data is on file at the Environmental Mutagen Information Center, Oak Ridge, Tenn.
Flag : Critical study for SIDS endpoint
24.07.2003 (15)

Type : Ames test
System of testing : Salmonella tester strains TA 1535, 1537, 98, 100
Test concentration : 10, 3, 1, 0.2, 0.04, 0.01 ul/plate
Cycotoxic concentr. : > 100 ul/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1978
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : Method used was plate incorporation assay based on Ames test methods consistent with OECD 471. A single test was run in triplicate at each dosage both with and without metabolic activation. The S-9 liver homogenates were prepared from male rats and given Arochlor 1254. All tester strains were obtained from Dr. B. Ames. Sterile DMSO was used as the solvent and a solvent control was employed of 20 uL/plate DMSO. Positive controls used were: 2-aminoanthracene, NaNo2 and 2 - nitrofluorene. A positive response was determined upon observation of a statistically significant dose-response increase in revertant colonies. Bartlett's test was used for pairwise comparison to controls and dose response determined using regression analysis for log-log straight lines; P<0.01 was used.A spot test was also conducted using a single dosage of 50 ul/plate with and without S-9. A toxicity test was run using TA-100 with and without S-9 at dosages of 100, 30, 10, 1, 0.3, and 0.1 ul/plate.
Result : No mutagenic changes were observed in any of the four tester strains used, with or without metabolic activation. No effects on background lawn were observed up to 100 ul/plate. No treatment-related mutagenic effects were observed in the Spot test, with or without metabolic activation, in any of the four tester strains.
Test substance : HB-40
Reliability : (2) valid with restrictions
Study limited to 4 of 5 Salmonella tester strains called for in test guidelines and used only a single test without confirmation. Highest test dose was below limit of toxicity. However, study confirms results of previously reported Salmonella test used to fulfill this HPV endpoint.
11.07.2003 (17)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Cytogenetic assay
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : i.p.
Exposure period : 24 hours

Doses	:	250, 1250, 2500 mg/kg
Result	:	negative
Method	:	OECD Guide-line 475 "Genetic Toxicology: In vivo Mammalian Bone Marrow Cytogenetic Test - Chromosomal Analysis"
Year	:	1986
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Dose levels selected based on both a range-find study followed by a pilot study where severe signs of toxicity and deaths (8/10) were seen at 5000 mg/kg test agent, the highest dose used in this study design. Six Fischer-344 rats/sex/time period were administered test agent in corn oil by intraperitoneal injection. Metaphase cells were collected from rat bone marrow (femur) at harvest times of 6, 12 and 24 hrs after treatment. Colchicine was administered 2 hr prior to sacrifice to arrest cells in c-metaphase. Marrow was exposed to hypotonic solution and fixed, cells and slides prepared and stained. All slides were coded before reading. Positive (Triethylene melamine) and negative (corn oil and untreated) controls were used for comparative purposes. Mitotic index was calculated based on counting of at least 1000 slides and chromosomal aberrations evaluated from at least 60 slides per animal per time point from the untreated control groups (male and female) and the 2,500 mg/kg test groups. All breaks, deletions, translocations and other changes were recorded. Mitotic Index, % chromosomally aberrant cells and frequency of chromosomal aberrations per cell were compared between treated vs control groups using ANOVA and Dunnett's test. P <0.05 was used.
Result	:	No significant differences in % chromosomally aberrant cells or frequency of chromosomal aberrations/cell were observed between the negative control group and any of the test article treated groups at any of the three time points investigated. The positive control performed as expected. No evidence of cytotoxicity was observed at any test level.
Test substance	:	Therminol 66
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

24.07.2003 (18)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	F0 & F1 Adults-premating through litter weaning (Fo) and postweaning (F1)
Frequency of treatm.	:	daily
Premating exposure period		
Male	:	FO- 14 weeks; F1- 18 weeks
Female	:	FO- 14 weeks; F1- 18 weeks
Duration of test	:	FO M/F - 167d; F1 M/F- 219d
No. of generation studies	:	2
Doses	:	30, 100, 300, 1000 ppm
Control group	:	yes, concurrent vehicle
NOAEL parental	:	= 1000 - ppm
NOAEL F1 offspring	:	= 1000 - ppm
NOAEL F2 offspring	:	= 1000 - ppm

Method	:	OECD Guide-line 416 "Two-generation Reproduction Toxicity Study"
Year	:	1991
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method : Test material was administered in the diet to groups of 30M and 30F rats of the F0 and F1 generations during a premating (70 days) growth period, and through the ensuing mating, gestation and lactation intervals (1 litter/generation) until day 21 post-partum. Dietary concentrations were analyzed by GC-FID weekly (all test levels first 4 weeks of the study, then one dose level weekly thereafter) to establish stability, homogeneity of mixing and target concentration accuracy. Body weights were recorded weekly for F0 and F1M. For F0 and F1 F wts were recorded weekly through the growth period and up to mating, then resumed after mating until sacrifice. Food consumption was recorded weekly for F0 and F1 M from study start up to mating, then resumed after mating through study term. Food consumption for adult females F0 and F1 was recorded weekly through the growth period and again after weaning of litters. Cageside observations for morbidity and mortality were made weekly, as well as daily observations of clinical signs. Temperature, humidity and light-dark cycles were controlled. F0 and F1 adults were sacrificed following weaning of their respective litters and given a gross postmortem examination. Reproductive tissues (testes, epididymides,seminal vesicles,uterus,vagina, mammary glands, prostate, ovaries) and selected other tissues (liver, pituitary, skin, and all gross lesions) were evaluated histopathologically for all control and high dose animals. Pups delivered to F0 and F1 females were evaluated for growth, survival and external irregularities during lactation days 0, 4, 7, 14 and 21. F1 pups not selected for the adult generation were sacrificed and given a gross postmortem exam. Body weights and changes, food consumption, gestation length and number of offspring were analyzed using ANOVA techniques followed by Dunnet's Test for parametric parameters and Kruskal-Willis test, Jonckheere or Mann-Whitney methods for nonparametric analysis. Mortality and pregnancy rates, fetal and mating indices and pup survival were analyzed using uncorrected Chi-square. Fisher's Exact test was used to statistically evaluate microscopic lesions. The level of significance was reported at both the 5% and 1% levels.

Result : No Adverse reproductive effects were observed in adult rats or their offspring up to the highest dose tested, i.e. 1000 ppm, the reproductive NOAEL for this study.

Small, statistically significant decreases in body weights were observed in High Dose (1000 ppm) F0 males during the last three weeks on test (mean wts 94% of control) and in F1a dams of the same dose group (mean weights 93% of control) during lactation days 0-7. Food consumption was statistically reduced in 1000 ppm F0 females during the first 2 weeks of gestation. These minor deviations from the norm are not considered sufficiently severe to constitute an adverse effect. Thus, the NOAEL for non-reproductive toxicity is considered 1000 ppm.

No treatment-related effects were noted in mating or fertility indices nor were any microscopic lesions attributable to treatment observed in reproductive organs (and other tissues) examined microscopically.

Test substance : Terminol 66; Daily average group mean dosages were calculated based on raw data for food consumption and body weight and were as follows:
Group (PPM): 30 100 300 1000

F0 males - 1.8, 6.1, 18.5 62.0 mg/kg/day
F0 females - 2.5, 8.3, 42.2, 81.2 mg/kg/day

F1 males - 1.9, 6.1, 18.2, 63.1 mg/kg/day
F1 females - 2.4, 8.1, 24.3, 80.6 mg/kg/day

Reliability : (2) valid with restrictions

Hematology, clinical chemistry, FOB and organ weights not conducted in this study, although all parameters were measured in subchronic study cited in this data package. Study itself sufficient to adequately judge fertility and reproductive indices.

Flag : Critical study for SIDS endpoint
24.07.2003 (19)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Solutia Technical report. THERMINOL 66. 03. 10-7 (5/03).

(2) Solutia Study No. MO20020690. 1982. Vapor Pressure of MXP-2020 at Ambient Temperature.

(3) Solutia Study no. MO-77-625. 1977. Comparison of Environmental Properties of CERECLOR 42 and SANTOSOL 340.

(4) Solutia Study no. MO-95-248. 1995. Aqueous Solubility of SANTOTHERM 66.

(5) Solutia Study No. MO20020691. 1982. Sunlight photolysis screening of MXP-2020.

(6) EPISUITE v. 3.10, US Environmental Protection Agency (2000).

(7) Solutia Study no. MO20020693. 1971. Biodegradation testing of Isopropylated Biphenyl (MIBP) and HB-40.

(8) Solutia Study no. AB-79-135a. 1979. Acute toxicity of Therminol 66 to Fathead Minnows (Pimephales promelas).

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(10) EPA's ECOSAR model (v. 0.99g). EPISUITE v. 3.10. US EPA (2000).

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(14) Solutia study no. ML19790079. 1979. Acute Oral Toxicity of HB-40 Plasticizer in Rats.

(15) Clark, CR, TC Marshall, BS Merickel, A Sanchez, DG Brownstein and CH Hobbs, 1979. Toxicological Assessment of Heat Transfer Fluids Proposed for Use in Solar Energy Applications. Toxicol. Appl. Pharmacol. 51:529-535.

(16) Solutia study no. BD19840360. 1984. Three Month Oral Toxicity Feeding Study in Rats with THERMINOL 66.

(17) Solutia Study no. DA-78-184. 1978. Salmonella Mutagenicity Assay of HB 40.

(18) Solutia Study no. SR-84-415. 1986. An Assessment of the Mutagenic Potential of THERMINOL 66 Utilizing the Acute In Vivo Rat Bone Marrow Cytogenetics Assay.

(19) Solutia Study no. ML-90-135. 1991. Two Generation Reproduction Study of THERMINOL 66 Heat Transfer Fluid in the Diet of Albino Rats.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT